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Final Report for PRF Grant 371-G Thermal Transition Probabilities in High Resolution Nuclear Magnetic Resonance

by

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This grant was used to initiate a program whose objective is the detailed characterization of nuclear spin relaxation in liquids and gases. Long range support for this program has been obtained from the National Science Foundation, and this research has been continued under NSF Grant GP-4299 titled "Nuclear Magnetic Relaxation."

The research funds were used to partially finance the construction of a frequency sweep proton-proton double resonance system. This system was made compatible with the already existing Varian DP-60 NMR spectrometer. The field-frequency lock circuit used is of the type described by Noggle[1] and was constructed by Research Systems, Inc.[2]

The fundamental problem in both nuclear spin relaxation and nuclear magnetic double resonance is that of a single nucleus of spin - 1/2. The power and relaxation relationships for this problem were investigated both theoretically and experimentally using the instrumentation described above. The double resonance spectrum for a single nucleus of spin - 1/2 is unusual in that both absorption and emission occur as the spectral features are recorded. The theoretical description was developed using both perturbation theory and the Bloch equations. The perturbation theory correctly predicted all experimental features except line shapes and saturation effects. The description in terms of the Bloch equations predicted all experimental features and has provided a detailed physical picture of the experiment.

The analysis showed that when the strong rf field is not in the immediate vicinity of the Larmor frequency the macroscopic moment is aligned with an "effective" field defined in a rotating coordinate system. When the strong rf field is at the Larmor frequency the macroscopic moment is perpendicular to the effective field. This produces considerable changes in line shapes and intensities as the strong rf is varied about the Larmor frequency. The spectrum in this region is sensitive to the relaxation times and provides a steady state method for measurement of relaxation times of the order of one second. The theoretical analysis was confirmed by experiment. This work was accepted for publication as an article in the Journal of Chemical Physics, and the financial support of this grant was acknowledged[3].

References

1. J. H. Noggle, "Spin Decoupler for NMR", Rev. Sci. Instr. 35, 1166 (1964).
2. Research Systems, Inc., 236 Grove St., Lexington, Massachusetts.
3. S. L. Gordon, "Nuclear Magnetic Double Resonance of a Single Nucleus of Spin - 1/2", J. Chem. Phys. (to be published).